

AN EXPLICIT FORMULA RELATING STIELTJES CONSTANTS AND LI'S NUMBERS

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ABSTRACT. In this paper we present a new formula relating Stieltjes numbers γ_n and Laurent coefficients η_n of logarithmic derivative of the Riemann's zeta function. Using it we derive an explicit formula for the oscillating part of Li's numbers $\tilde{\lambda}_n$ which are connected with the Riemann hypothesis.

1. INTRODUCTION

First recall some basic definitions and conventions. The Stieltjes constants γ_n are essentially the coefficients in the Laurent expansion of the Riemann zeta function about $s = 1$:

$$(1.1) \quad \zeta(s+1) = \frac{1}{s} + \sum_{n=0}^{\infty} \gamma_n s^n$$

(Sometimes another convention is adopted. It differs from the above by the factor $(-1)^n/n!$) It is well known that zeta has a single simple pole at $s = 1$ with residue 1 which is evident from (1.1).

Other useful coefficients η_n are these which appear in the Laurent expansion of the logarithmic derivative of zeta about $s = 1$:

$$(1.2) \quad -\frac{\zeta'}{\zeta}(s+1) = \frac{1}{s} + \sum_{n=0}^{\infty} \eta_n s^n$$

It can be shown that [1]

$$(1.3) \quad \gamma_n := \frac{(-1)^n}{n!} \lim_{x \rightarrow \infty} \left(\sum_{k \leq x} \frac{(\log k)^n}{k} - \frac{(\log x)^{n+1}}{n+1} \right)$$

$$(1.4) \quad \eta_n := \frac{(-1)^n}{n!} \lim_{x \rightarrow \infty} \left(\sum_{k \leq x} \Lambda(k) \frac{(\log k)^n}{k} - \frac{(\log x)^{n+1}}{n+1} \right)$$

Date: 13 June 2004.

Key words and phrases. Li's criterion for the Riemann hypothesis, numerical methods in analytic number theory.

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where $\Lambda(k)$ denotes the von Mangoldt function (see e.g. [3], p. 50). It is related to the Riemann zeta function by

$$-\frac{\zeta'(s)}{\zeta(s)} = \sum_{n=2}^{\infty} \frac{\Lambda(n)}{n^s}$$

where $\Re s > 1$. It may be shown that $\Lambda(n)$ is zero unless n is a prime power: $n = p^k$, in which case $\Lambda(n)$ is $\log(p)$

However, the expansions (1.3) and (1.4) are slowly convergent and are therefore useless in numerical computations. Effective numerical algorithms for calculating γ_n were given by Keiper [4] and Kreminski [5]. An interesting recurrence relation involving both γ_n and η_n has been recently discovered by Coffey [2] (written here in our convention (1.1) and (1.3) concerning γ_n):

$$(1.5) \quad \eta_n = -(n+1)\gamma_n - \sum_{k=0}^{n-1} \eta_k \gamma_{n-k-1}$$

2. DERIVATION

Here are several initial relations obtained directly using (1.2):

$$(2.1) \quad \begin{aligned} \eta_0 &= -\gamma_0 \\ \eta_1 &= +\gamma_0^2 - 2\gamma_1 \\ \eta_2 &= -\gamma_0^3 + 3\gamma_0\gamma_1 - 3\gamma_2 \\ \eta_3 &= +\gamma_0^4 - 4\gamma_0^2\gamma_1 + 2\gamma_1^2 + 4\gamma_0\gamma_2 - 4\gamma_3 \\ \eta_4 &= -\gamma_0^5 + 5\gamma_0^3\gamma_1 - 5\gamma_0\gamma_1^2 - 5\gamma_0^2\gamma_2 + 5\gamma_1\gamma_2 + 5\gamma_0\gamma_3 - 5\gamma_4 \\ &\dots \end{aligned}$$

With growing n the number of terms in η_n increases as the so-called partition number.

At the first glance there seem to be some regularities in (2.1). Indeed, careful (and very tedious) inspection of the indices in γ s, their exponents, as well as the numerical coefficients reveals several simple rules:

- (1) Each η_n is a linear combination of products of powers of Stieltjes numbers with some numerical coefficient: $\pm A \gamma_i^{k_i} \gamma_j^{k_j} \dots \gamma_m^{k_m}$.
- (2) Every such term appears only once. More precisely, $\pm A \gamma_i^{k_i} \gamma_j^{k_j} \dots \gamma_m^{k_m}$ appears in η_n with $n = (i+1)k_i + (j+1)k_j + \dots (m+1)k_m$.
- (3) The sign of each term is determined by the sum of *all* exponents k_i : it is equal to $(-1)^p$, where $p = \sum_{i=0}^n k_i$.
- (4) The numerical coefficients A which appear in η_n may be obtained as follows. Let us discard for a while in each term power of γ_0 , i.e. $\gamma_0^{k_0}$, if there is one. It turns out that A contains two factors. The first is

$$\frac{n}{k_i!k_j!\dots k_m!}$$

and the other is

$$\prod_{i=s+1}^{q-2} (n-i)$$

where s is the sum of all indices of γ in a given product and q is the number of all γ s in the same product (in both cases γ s are counted according to their multiplicity and in both cases we neglect γ_0), i.e.

$$\begin{aligned} s &= ik_i + jk_j + \dots + mk_m \\ q &= k_i + k_j + \dots + k_m \end{aligned}$$

The above product may be further simplified:

$$\prod_{i=s+1}^{q-2} (n-i) = -(-1)^q \frac{\Gamma(s+q-n)}{\Gamma(s-n+1)} = \frac{\Gamma(n-s)}{\Gamma(n-s-q+1)}$$

where the last equality stems from the properties of the Pochhammer's symbol. According to (2) we have $n-s-q+1 = k_0+1$, and therefore $\Gamma(n-s-q+1) = k_0!$. The last step is equivalent to restoring the powers of γ_0 in the general term $\pm A \gamma_i^{k_i} \gamma_j^{k_j} \dots \gamma_m^{k_m}$.

Collecting all the above rules (1-4) together leads to the general expression for η as a function of appropriate γ s:

$$(2.2) \quad \boxed{\eta_{n-1} = n \sum_{k_i=0}^n \left[\Gamma(p) \delta_{n,r} \prod_{i=0}^n \frac{(-\gamma_i)^{k_i}}{k_i!} \right]}$$

where

$$(2.3) \quad \begin{aligned} p &\equiv p(k_0, k_1, \dots, k_n) = \sum_{i=0}^n k_i \\ r &\equiv r(k_0, k_1, \dots, k_n) = \sum_{i=0}^n (1+i) k_i \end{aligned}$$

and the sum (2.2) is performed over *all* combinations of integers $k_i = 0, 1, 2, \dots$ satisfying the constraints (2.3). This sum contains formally many terms, roughly $O(n^n)$, but, due to the Kronecker delta which picks out only appropriate terms (i.e. when $r = n$) and cuts off all the others, the number of non-zero terms is much smaller. This neat and concise relation (2.2) is in fact pretty sophisticated.

Formula (2.2) may be inverted. Writing down several initial expressions (by solving the quasi-linear system (2.1) with respect to γ_n) we get:

$$\begin{aligned}
 (2.4) \quad & -\eta_0 \\
 \gamma_1 &= \frac{1}{2} (+\eta_0^2 - \eta_1) \\
 \gamma_2 &= \frac{1}{3!} (-\eta_0^3 + 3\eta_0\eta_1 - 2\eta_2) \\
 \gamma_3 &= \frac{1}{4!} (+\eta_0^4 - 6\eta_0^2\eta_1 + 3\eta_1^2 + 8\eta_0\eta_2 - 6\eta_3) \\
 \gamma_4 &= \frac{1}{5!} (-\eta_0^5 + 10\eta_0^3\eta_1 - 15\eta_0\eta_1^2 - 20\eta_0^2\eta_2 + 20\eta_1\eta_2 + 30\eta_0\eta_3 - 24\eta_4) \\
 & \dots
 \end{aligned}$$

Again, several regularities are evident. When collected together in the same way as before they give:

$$(2.5) \quad \gamma_{n-1} = \sum_{k_i=0}^n \left[\delta_{n,r} \prod_{i=0}^n \frac{1}{k_i!} \left(\frac{-\eta_i}{1+i} \right)^{k_i} \right]$$

where r is given by the second relation (2.3). It should be emphasized that formulas (2.5) and (2.2), as well as (3.2) below, may be effectively implemented e.g. using *Mathematica* symbolic package (it is not trivial since the number of summations and products is variable):

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Table[{Subscript[\[Eta],n-1],
Factor[n*Sum[\Gamma[Sum[Subscript[k,i],{i,0,n}]]]*
KroneckerDelta[n,Sum[(1+i)*Subscript[k,i],{i,0,n}]]*
Product[(-Subscript[\[Gamma],i])^Subscript[k,i]/Subscript[k,i]!,{i,0,n}],
Evaluate[Apply[Sequence,Table[{Subscript[k,j],0,n},{j,0,n}]]]
]],{n,1,5}]

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where the Euler gamma function Γ above is slightly modified:

$$\Gamma[n_-] := \text{Gamma}[\text{If}[n == 0, 1, n]]$$

3. APPLICATIONS

It was shown elsewhere by the author [7] that the behavior of certain numbers $\tilde{\lambda}_n$ with growing n is crucial for the Riemann hypothesis to be true. Now using

$$(3.1) \quad \tilde{\lambda}_n = - \sum_{j=1}^n \binom{n}{j} \eta_{j-1}$$

together with (2.2) we get

$$(3.2) \quad \tilde{\lambda}_n = - \sum_{k_i=0}^n \left[\Gamma(p) \binom{n}{r} r \prod_{i=0}^n \frac{(-\gamma_i)^{k_i}}{k_i!} \right]$$

which explicitly expresses the oscillating part of Li's numbers using Stieltjes constants. Similarly as in (2.2), due to the binomial coefficient there are in fact many redundant terms in (3.2) which are identically zero, i.e. always when r is greater than n . Those which are non-zero ($r \leq n$) give:

$$(3.3) \quad \begin{aligned} \tilde{\lambda}_1 &= \gamma_0 \\ \tilde{\lambda}_2 &= 2\gamma_0 - \gamma_0^2 + 2\gamma_1 \\ \tilde{\lambda}_3 &= 3\gamma_0 - 3\gamma_0^2 + \gamma_0^3 + 6\gamma_1 - 3\gamma_0\gamma_1 + 3\gamma_2 \\ \tilde{\lambda}_4 &= 4\gamma_0 - 6\gamma_0^2 + 4\gamma_0^3 - \gamma_0^4 + 12\gamma_1 - 12\gamma_0\gamma_1 + 4\gamma_0^2\gamma_1 - 2\gamma_1^2 \\ &\quad + 12\gamma_2 - 4\gamma_0\gamma_2 + 4\gamma_3 \\ &\dots \end{aligned}$$

With growing n the number of terms in $\tilde{\lambda}_n$ increases as the summatory function for partition number, i.e. faster than in the case of (2.2).

4. DISCUSSION

The distribution of values for various terms which contribute to (3.3) is very nonuniform. When $n \rightarrow \infty$ the majority of values is concentrated near zero. In Figure 1 there are eight histograms for $n = 3, 4, \dots, 10$. The shape of these histograms is roughly symmetrical about zero but it is just the slight departure from symmetry which contributes to $\tilde{\lambda}_n$.

(Figure 1 about here)

The fundamental problem, equivalent to the Riemann hypothesis itself is whether the oscillating part of Li's numbers $\tilde{\lambda}_n$ is bounded by the trend $\bar{\lambda}_n$ which grows asymptotically as:

$$\bar{\lambda}_n \sim \frac{1}{2} (1 + n \ln n) + cn$$

where (cf. [8], [6]):

$$c = \frac{1}{2} (\gamma - 1 - \ln 2\pi)$$

Acknowledgment: I would like to thank dr. Michael Trott, Wolfram Research, for pointing my attention to a typographical error in a formula as well as for checking the calculations using *Mathematica*.

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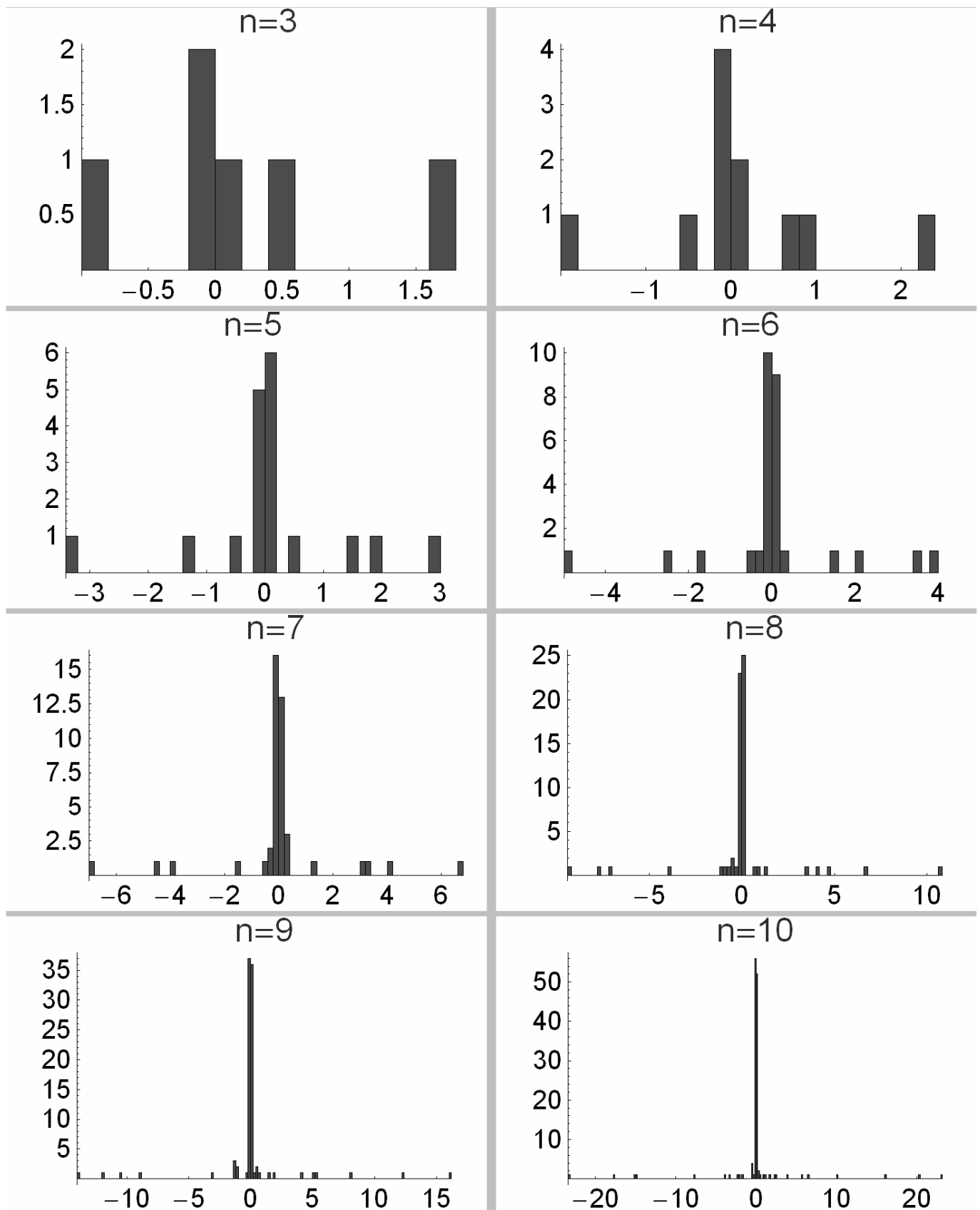


Figure 1.

Distribution of terms in formula (3.2) for $n=3,4,\dots,10$. These terms sum up to the oscillating part of λ_n . As usual, the base of each rectangle is equal to the width of the class interval and its height is proportional to the number of data values in the class. The base is always equal to $1/5$. Note changes in the horizontal scale when n increases.